Density-matrix functional theory of strongly-correlated lattice fermions

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Abstract

A density functional theory (DFT) of lattice fermion models is presented, which uses the single-particle density matrix γ_{ij} as basic variable. A simple, explicit approximation to the interaction-energy functional $W[\gamma]$ of the Hubbard model is derived from exact dimer results, scaling properties of $W[\gamma]$ and known limits. Systematic tests on the one-dimensional chain show a remarkable agreement with the Bethe-Ansatz exact solution for all interaction regimes and band fillings. New results are obtained for the ground-state energy and charge-excitation gap in two dimensions. A successful description of strong electron correlations within DFT is achieved.

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I. INTRODUCTION

First principles methods and many-body lattice models are the two main theoretical approaches to the electronic properties of matter. From the first-principles perspective, the major breakthrough in the last decades has been Hohenberg-Kohn-Sham's (HKS) density-functional theory (DFT) and the derived powerful methods of electronic-structure calculation.[1] Despite their unparalleled success in an extremely wide variety of problems, current implementations of DFT have still serious difficulties in accounting for phenomena that involve strong electron correlations as observed, for example, in heavy-fermion materials, Mott insulators or high-T_c superconductors.[2] Being in principle an exact theory, the limitations of DFT have to be ascribed to the approximations used for the interaction-energy functional $W[\rho(\vec{r})]$ and not to the underlying formalism. The development of new functionals improving the description of strong correlation effects is therefore a major current theoretical challenge.

On the other side, the physics of strongly-correlated Fermi systems is intensively studied in the framework of parametrized lattice models (e.g., Hubbard, Anderson, etc.) by using specific leading-edge many-body techniques.[2] Taking into account the universality of DFT, and its demonstrated efficiency in complex *ab initio* calculations, it is quite remarkable that only few investigations have been concerned so far with applying the concepts of DFT to the lattice models describing strongly correlated fermions.[3,4,5,6] In fact, already from a formal standpoint, one may expect that DFT with an appropriate Ansatz for W should be a particularly valuable many-body approach to lattice models, thus becoming a subject of theoretical interest on its own. Moreover, DFT studies on simpler universal models also provide useful new insights relevant to first principles calculations,[1] particularly since in some cases the exact solution of the many-body problem is available.[2]

The purpose of this paper is to extend the scope of DFT to the description of strong electron correlations in lattice Hamiltonians and to demonstrate quantitatively for the first time the performance of lattice density-functional theory (LDFT) in one-dimensional (1D) and two-dimensional (2D) systems. Sec. II presents concisely the basic formalism of LDFT. In this framework the ground-state properties are obtained from the solution of exact self-consistent equations that involve derivatives of the interaction-energy functional $W[\gamma]$ with respect to the single-particle density matrix γ. In Sec. III the dependence of W on the

nearest-neighbor (NN) density-matrix element γ_{12} is analyzed and a simple explicit approximation to $W(\gamma_{12})$ is derived for the Hubbard model. Sec. IV discusses representative applications of this *Ansatz*. First, the accuracy of the method is demonstrated by comparison with available exact results on the 1D Hubbard model. New results are then discussed, particularly concerning the ground-state energy and charge-excitation gap in 2D lattices. Finally, Sec. V summarizes our conclusions.

II.   LATTICE DENSITY-FUNCTIONAL THEORY

In order to be explicit we focus on the Hubbard model which is expected to capture the main physics of lattice fermions in a narrow energy band. The Hamiltonian

$$H = \sum_{\langle i,j\rangle\sigma} t_{ij}\hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma} + U\sum_{i} \hat{n}_{i\downarrow}\hat{n}_{i\uparrow}, \tag{1}$$

includes nearest neighbor (NN) hoppings t_{ij}, and an on-site interactions U ($\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^{\dagger}\hat{c}_{i\sigma}$). The importance of electron correlations is controlled by one parameter, namely, the ratio U/t. The hopping integrals t_{ij} are defined by the lattice structure (typically, $t_{ij} = -t < 0$ for NN ij) and thus play the role given in conventional DFT to the external potential $V_{ext}(\vec{r})$. Consequently, in LDFT the single-particle density matrix γ_{ij} replaces the density $\rho(\vec{r})$ as basic variable, since the hopping integrals t_{ij} are nonlocal in the sites.[4] The situation is similar to the density-matrix functional theory proposed by Gilbert for the study of nonlocal pseudopotentials.[7,8]

The ground-state energy E_{gs} and density-matrix γ_{ij}^{gs} are determined by minimizing the energy functional

$$E[\gamma] = E_K[\gamma] + W[\gamma] \tag{2}$$

with respect to γ_{ij}.[4] The first term

$$E_K[\gamma] = \sum_{ij} t_{ij}\gamma_{ij} \tag{3}$$

is the kinetic energy associated with the electronic motion in the lattice. The second term is Levy's interaction-energy functional[9] given by

$$W[\gamma] = \min\left[U\sum_{i}\langle\Psi[\gamma]|\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}|\Psi[\gamma]\rangle\right], \tag{4}$$

where the minimization runs over all N-particle states $|\Psi[\gamma]\rangle$ satisfying

$$\langle\Psi[\gamma]|\sum_\sigma \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}|\Psi[\gamma]\rangle = \gamma_{ij} \tag{5}$$

for all i and j.[4,5,6,7] $W[\gamma]$ represents the minimum interaction energy compatible with a given γ_{ij}. It is a universal functional in the sense that it is independent of t_{ij}. However, note that it still depends on the type of model interaction, on the number of electrons N_e or band filling $n = N_e/N_a$, and on the number of sites N_a.[10]

$E[\gamma]$ is minimized by expressing $\gamma_{ij} = \gamma_{ij\uparrow}+\gamma_{ij\downarrow}$ in terms of its eigenvalues $\eta_{k\sigma}$ (occupation numbers) and eigenvectors $u_{ik\sigma}$ (natural orbitals) as

$$\gamma_{ij\sigma} = \sum_k u_{ik\sigma}\eta_{k\sigma}u_{jk\sigma}^* \ . \tag{6}$$

Introducing Lagrange multipliers μ and $\lambda_{k\sigma}$ ($\varepsilon_{k\sigma} = \lambda_{k\sigma}/\eta_{k\sigma}$) to impose the usual constraints $\sum_{k\sigma}\eta_{k\sigma} = N_e$ and $\sum_i |u_{ik\sigma}|^2 = 1$, one obtains the eigenvalue equations

$$\sum_j \left(t_{ij} + \frac{\partial W}{\partial\gamma_{ij\sigma}}\right) u_{jk\sigma} = \varepsilon_{k\sigma}u_{ik\sigma} \tag{7}$$

with $\varepsilon_{k\sigma} < \mu$ ($\varepsilon_{k\sigma} > \mu$) if $\eta_{k\sigma} = 1$ ($\eta_{k\sigma} = 0$), and

$$\varepsilon_{k\sigma} = \mu \quad \text{if} \quad 0 < \eta_{k\sigma} < 1 \ . \tag{8}$$

In Eq. (7) self-consistency is implied by the dependence of $\partial W/\partial\gamma_{ij\sigma}$ on $\eta_{k\sigma}$ and $u_{ik\sigma}$. The present formulation is analogous to well-known results of density-matrix functional theory in the continuum.[7] However, notice the fundamental differences with respect to the KS-like approach proposed in Ref.[4], which assumes non-interacting v-representability, and where only integer occupations are allowed. The importance of fractional orbital occupations to the description of electron correlations within density-matrix functional theory has already been stressed by Gilbert.[7] In particular for the Hubbard model, one observes that $0 < \eta_{k\sigma} < 1$ for all k, except in very special situations such as $U/t = 0$ or the fully-polarized ferromagnetic state. This can be understood from perturbation-theory arguments —none of the $\eta_{k\sigma}$ is a good quantum number for $U/t \neq 0$— and has been explicitly demonstrated in exact solutions for finite clusters or the 1D chain.[11] Therefore, the case (8) is the only relevant one in general and all $\varepsilon_{k\sigma}$ in Eq. (7) must be degenerate. Consequently,

$$t_{ij} + \frac{\partial W}{\partial\gamma_{ij\sigma}} = \delta_{ij}\,\mu \tag{9}$$

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for all i and j. Note that approximations of W in terms of diagonal γ_{ii} alone can never yield such a behavior.[8]

At this point it is important to observe that the general functional, valid for all lattice structures and for all types of hybridizations, can be simplified at the expense of universality if the hopping integrals are short ranged. For example, if only NN hoppings are considered, E_K is independent of γ_{ij} for pairs of sites ij that are not NN's. In this case, the constraints $\langle \Psi[\gamma]| \sum_\sigma \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} |\Psi[\gamma]]\rangle = \gamma_{ij}$ in Eqs. (4) and (5) need to be imposed only for $i = j$ and for NN ij. This allows to reduce drastically the number of variables and simplifies considerably the search for practical approximations to W. Moreover, in periodic lattices the ground-state γ^{gs}_{ij} is a translational invariant. In order to determine E_{gs} and γ^{gs}_{ij}, one may then set $\gamma_{ii} = n = N_e/N_a$ for all sites i, and $\gamma_{ij} = \gamma_{12}$ for all NN pairs ij. Thus, the interaction energy can be regarded as a simple function $W(\gamma_{12})$ of the density-matrix element between NN's. It should be however noted that this also implies that W loses its universal character, since the NN map and the resulting dependence of W on γ_{12} are in principle different for different lattice structures.[6]

III.   INTERACTION-ENERGY FUNCTIONAL FOR THE HUBBARD MODEL

Given a self-consistent scheme that implements the variational principle, the challenge is to find a good, explicit approximations to the interaction-energy functional. $W[\gamma]$ may be determined exactly for small clusters by using numerical methods that perform the constrained minimization explicitly.[6] For a Hubbard dimer with $N_e = N_a = 2$ a straightforward analytical calculations yields

$$\frac{W(\gamma_{12})}{N_a} = \frac{U}{4}\left(1 - \sqrt{1 - \gamma_{12}^2}\right) , \tag{10}$$

which represents the minimum average number of double occupations for a given degree of electron delocalization, i.e., for a given γ_{12} ($U > 0$). Despite its simplicity, Eq. (10) already includes the fundamental interplay between electron delocalization and charge fluctuations, and provides useful insights on several general properties of $W(\gamma_{12})$ that are valid for arbitrary lattices:

(i) The domain of definition of $W(\gamma_{12})$ is limited by the pure-state representability of γ_{12}. In fact, $\gamma_{12} \leq \gamma^0_{12} = 1$, where γ^0_{12} corresponds to the extreme of the kinetic energy (maximum

degree of delocalization) and thus to the $U = 0$ ground-state for a given lattice and a given n.

(ii) For $\gamma_{12} = \gamma_{12}^0$, the underlying electronic state $\Psi[\gamma_{12}^0]$ is a single Slater determinant and therefore $W(\gamma_{12}^0) = E_{\text{HF}} = n^2 U/4$, where E_{HF} is the Hartree-Fock energy. Moreover, $\partial W/\partial \gamma_{12} = \infty$ for $\gamma_{12} = \gamma_{12}^0$, since $\gamma_{12}^{gs} < \gamma_{12}^0$ already for arbitrary small U/t, as expected from perturbation theory.

(iii) Starting from $\gamma_{12} = \gamma_{12}^0$, $W(\gamma_{12})$ decreases monotonically with decreasing γ_{12} reaching its lowest possible value, $W = 0$, for $\gamma_{12} = \gamma_{12}^\infty$ ($\gamma_{12}^\infty = 0$ for $n = 1$). The fact that W decreases with decreasing $|\gamma_{12}|$ shows that the correlation-induced reduction of the Coulomb energy is obtained at the expense of electron delocalization.

(iv) γ_{12}^∞ represents the largest NN bond order that can be obtained under the constraint of vanishing Coulomb energy. A lower bound for γ_{12}^∞ is given by the bond order γ_{12}^{FM} in the fully-polarized ferromagnetic state which is formed by occupying the N_e lowest single-particle states of the same spin ($n \leq 1$). Note that the ground-state γ_{12}^{gs} always satisfies $\gamma_{12}^\infty \leq \gamma_{12}^{gs} \leq \gamma_{12}^0$ even though, for $n \neq 1$, it is possible to construct N_e-electron states having $|\gamma_{12}| < |\gamma_{12}^\infty|$.

In order to derive a simple approximation to $W(\gamma_{12})$ that preserves the previous general properties we take advantage of its scaling properties. Exact numerical studies[6] have shown that $W(\gamma_{12})$ depends weakly on N_e, N_a and lattice structure if it is measured in units of E_{HF} and if γ_{12} is scaled within the relevant domain of representability $[\gamma_{12}^\infty, \gamma_{12}^0]$. Physically, this means that the relative change in W associated to a given change in the degree of electron localization $g_{12} = (\gamma_{12} - \gamma_{12}^\infty)/(\gamma_{12}^0 - \gamma_{12}^\infty)$ can be regarded as nearly independent of the system under study. A good general approximation to $W(\gamma_{12})$ can then be obtained by applying such a scaling to the functional dependence extracted from a simple reference system which already contains the fundamental relationship between localization and correlation. We therefore derive an approximate $W(\gamma_{12})$ taking its functional dependence from the exact result for the Hubbard dimer given by Eq. (10). In this way one obtains

$$W(\gamma_{12}) = E_{\text{HF}} \left(1 - \sqrt{1 - \frac{(\gamma_{12} - \gamma_{12}^\infty)^2}{(\gamma_{12}^0 - \gamma_{12}^\infty)^2}} \right) , \qquad (11)$$

where E_{HF}, γ_{12}^0 and γ_{12}^∞ are system specific [see (i)–(iv) above]. In practice, γ_{12}^∞ may be approximated by the ferromagnetic fully-polarized γ_{12}^{FM} which is calculated, as γ_{12}^0, by integration of the single-particle spectrum.
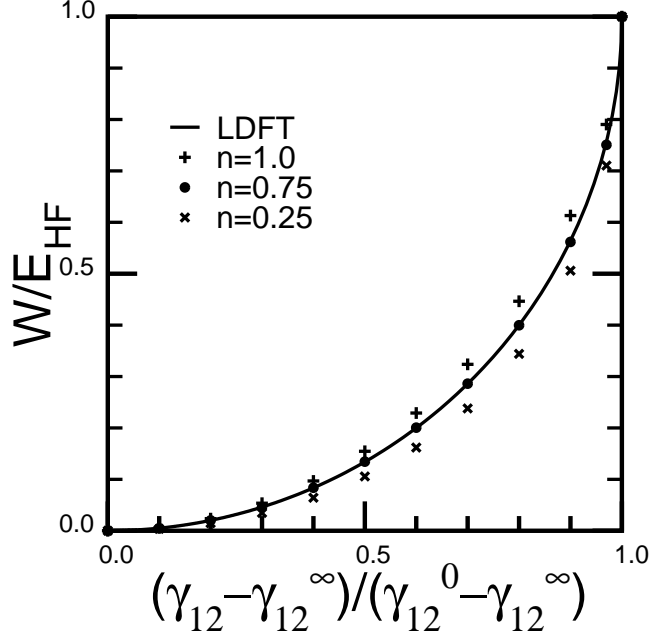
FIG. 1: Interaction energy $W(\gamma_{12})$ of the one-dimensional (1D) Hubbard model as a function of the degree of electron delocalization $(\gamma_{12} - \gamma_{12}^\infty)/(\gamma_{12}^0 - \gamma_{12}^\infty)$. The symbols refer to exact results for different band fillings n and the solid curve to Eq. (11).

Fig. 1 compares Eq. (11) with the exact $W_{ex}(\gamma_{12})$ of the 1D Hubbard chain which is derived from the Bethe-Ansatz solution.[11] One observes that the proposed approximation follows $W_{ex}(\gamma_{12})$ quite closely all along the crossover from weak correlations (large W/U and γ_{12}) to strong correlations (small W/U and γ_{12}). This is remarkable, taking into account the simplicity of Eq. (11) and the strong band-filling dependence of E_{HF}, γ_{12}^0, and γ_{12}^∞. The quantitative discrepancies between Eq. (11) and $W_{ex}(\gamma_{12})$ remain small in the complete domain of representability of γ and for all band fillings: $|W - W_{ex}|/E_{\mathrm{HF}} \leq 0.063$ for all γ_{12} and n. Consequently, a good general performance of the method can be expected already at this stage. In the following section several applications of LDFT are discussed by using Eq. (11) as approximation to the interaction-energy functional.

IV.   RESULTS AND DISCUSSION

In Fig. 2 the ground-state energy E_{gs} of the 1D Hubbard model is given as a function of band filling n for different values of Coulomb repulsion U/t. Comparison between LDFT and the Bethe-Ansatz exact solution shows a very good agreement. It is interesting to
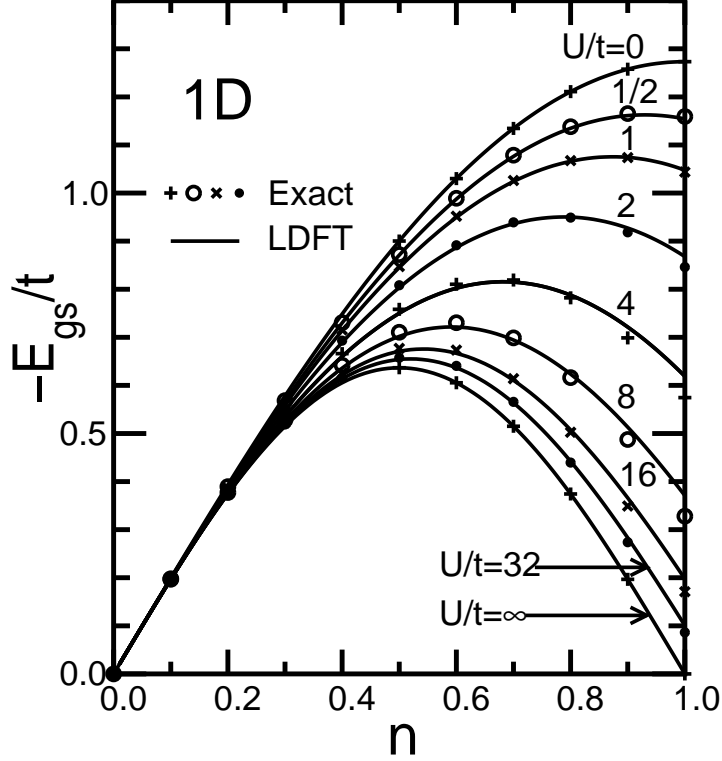
FIG. 2: Ground-state energy E_{gs} of the 1D Hubbard model as a function of band filling n for different Coulomb repulsions U/t. The solid curves refer to the present lattice density-functional theory (LDFT) and the symbols to the Bethe-Ansatz exact solution.[11]

observe that the accuracy of the calculated E_{gs} is not the result of a strong compensation of errors since a similar accuracy is achieved for the kinetic and Coulomb energies separately. Indeed, as shown in Fig. 3, both local moments $S_i^2 = 3\langle(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2\rangle$ and kinetic-energy renormalizations are also very well reproduced as a function of U/t. Moreover, notice that no artificial symmetry breaking is required in order to describe correctly the correlation-induced localization, as it is often the case in other approaches (e.g., antiferromagnetic spin-density wave for $n = 1$). For $n \leq 0.8$, the LDFT results are almost indistinguishable from the exact ones. Even the largest quantitative discrepancies, found for $n = 1$ and intermediate U/t, are acceptably small (e.g., $|E_{gs} - E_{gs}^{ex}|/t = 0.044$ for $U/t = 4$). For $U \gg t$ and $n = 1$ we obtain $E_{gs} \simeq -\alpha t^2/U$ with $\alpha \simeq 3.24$ while the exact result is $\alpha = 4\ln 2 \simeq 2.77$. The error in the coefficient α can be corrected by including in Eq. (11) a 4th-order term in g_{12} which provides in addition with a systematic improvement for all values of the interaction strength ($|E_{gs}^{ex} - E_{gs}|/|E_{gs}^{ex}| < 0.02$ for all U/t).[12]
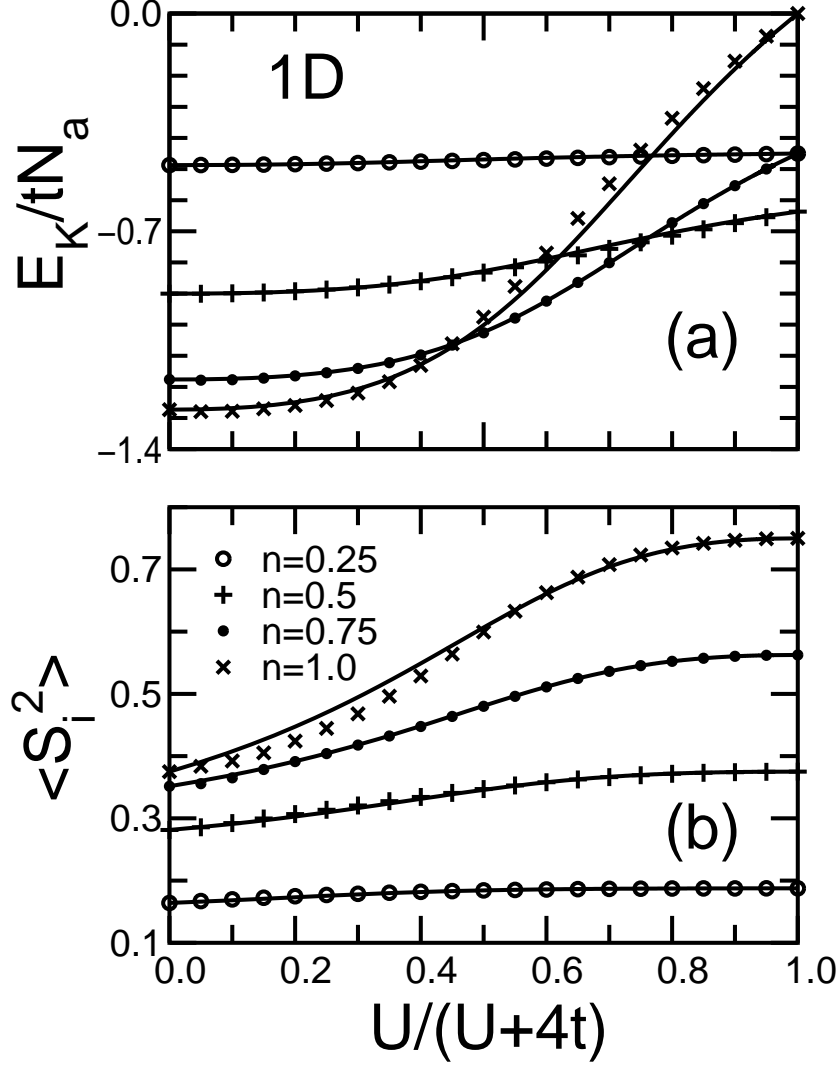
FIG. 3: (a) Kinetic energy E_K and (b) local magnetic moments $S_i^2 = 3\langle(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2\rangle$ of the 1D Hubbard model as a function of Coulomb repulsion U/t for different band fillings n as indicated in the inset of subfigure (b). The solid curves correspond to the present LDFT and the symbols to the Bethe-Ansatz exact solution.[11]

Fig. 4 shows E_{gs} of the 2D square lattice as a function of U/t for representative band-fillings n. The LDFT results cover the complete range of model parameters involving essentially analytic calculations. As shown in Fig. 5, good agreement is obtained with far more demanding ground-state quantum Monte Carlo (QMC) studies[13] for $U/t = 4$. The reliability of LDFT in 2D systems is confirmed by comparison with exact Lanczos diagonalizations on small clusters of the square and triangular lattices. In the inset of Fig. 5 we consider for example a $N_a = 3 \times 4$ cluster of the square lattice with periodic bound-
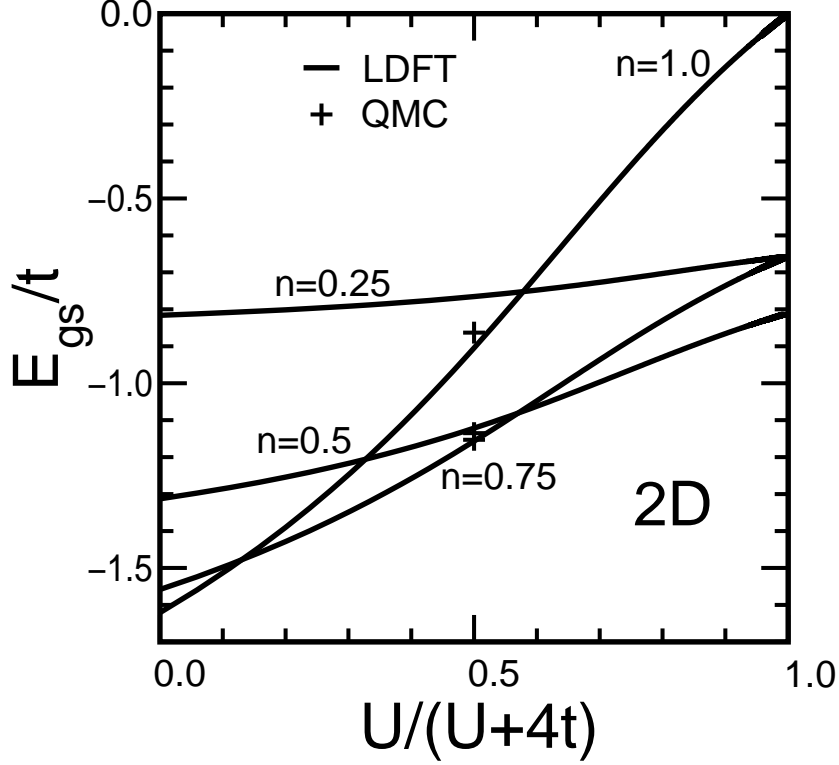
FIG. 4: Ground-state energy E_{gs} of the Hubbard model on the 2D square lattice as a function of Coulomb-repulsion strength U/t and for different band fillings n. The solid curves refer to the present LDFT and the crosses to quantum Monte Carlo (QMC) calculations.[13]

ary conditions and $N_e = N_a$. Like in the 1D case, the overall performance is very good, with the largest quantitative discrepancies being observed for intermediate values of U/t. For instance, for $U/t = 1$ one obtains $|E_{gs} - E_{gs}^{ex}|/|E_{gs}^{ex}| = 4.4 \times 10^{-3}$, and for $U/t = 4$ $|E_{gs} - E_{gs}^{ex}|/|E_{gs}^{ex}| = 9.8 \times 10^{-2}$. Results with similar precision are found for a the triangular 2D lattice. In this case, using also a $N_a = N_e = 3 \times 4$ cluster with periodic boundary conditions, we find $|E_{gs} - E_{gs}^{ex}|/|E_{gs}^{ex}| = 1.7 \times 10^{-4}$ for $U/t = 1$, and $|E_{gs} - E_{gs}^{ex}|/|E_{gs}^{ex}| = 6.6 \times 10^{-2}$ for $U/t = 4$. For both lattice structures $|E_{gs} - E_{gs}^{ex}|$ decreases quite rapidly away from half-band filling as in the 1D chain (see Fig. 2). LDFT, combined with Eq. (11) for $W(\gamma_{12})$, provides a correct description of electron correlations in different dimensions and lattice structures.

The charge-excitation or band gap

$$\Delta E_c = E_{gs}(N_e + 1) + E_{gs}(N_e - 1) - 2E_{gs}(N_e) \qquad (12)$$

is a property of considerable interest in strongly correlated systems which measures the
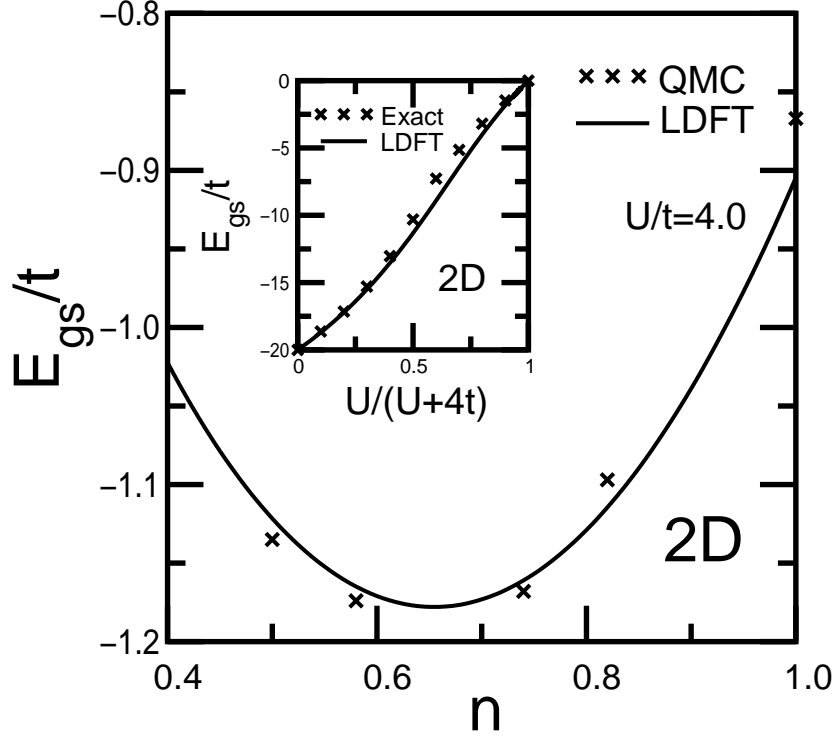
FIG. 5: Ground-state energy E_{gs} of the Hubbard model on the 2D square lattice as a function of band filling n for $U/t = 4$. The solid curve refers to the present lattice density-functional theory (LDFT) and the crosses to quantum Monte Carlo (QMC) calculations[13]. In the inset figure LDFT is compared to exact Lanczos diagonalizations for a $N_a = 3 \times 4$ cluster of the 2D square lattice with periodic boundary conditions. Results are here given as a function of U/t at half-band filling $(n = N_e/N_a = 1)$.

insulating or metallic character of the electronic spectrum as a function of U/t and n. It can be directly related to the discontinuity in the derivative of the kinetic and correlation energies per site with respect to electron density n.[14] Therefore, the determination of ΔE_c constitutes a much more serious challenge than the calculation of E_{gs}, particularly in the framework of a density-functional formalism. At half-band filling, $\Delta E_c = 0$ in the uncorrelated limit $(U/t = 0)$ and it increases with increasing U/t. For $U/t \to \infty$, $\Delta E_c \to U + E_b$ where E_b is the energy of the bottom of the single-particle band ($E_b = -4t$ for a 1D chain and $E_b = -8t$ for the 2D square lattice). Fig. 6 presents LDFT results for ΔE_c in 1D and 2D Hubbard models ($n = 1$). Comparison with the Bethe-Ansatz results[11] and with available QMC calculations[13] shows a good overall agreement. However, a more detailed analysis reveals that in the 1D case the gap is significantly overestimated for $U/t \ll 1$. Here we obtain
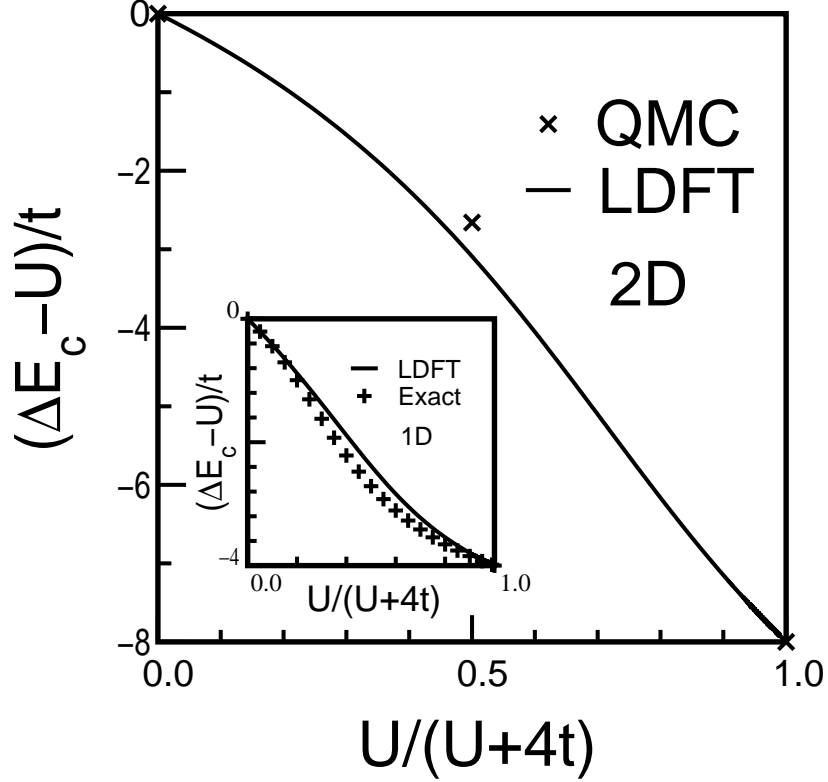
FIG. 6: Charge excitation gap ΔE_c of the 2D Hubbard model (square lattice, $n = 1$). In the inset results are given for the 1D chain. The solid curves refer to the present LDFT and the crosses to QMC calculations (2D, $U/t = 4$) or to exact Bethe-Ansatz results (1D).[11,13]

$\Delta E_{\mathrm{c}} \propto (U/t)^2$, while the exact solution shows that for the infinite chain ΔE_{c} increases much more slowly, namely, exponentially in $-t/U$. This discrepancy reflects the difficulty to describe long range-effects using an interaction-energy which functional dependence is derived from the dimer. Thus, it is possible that a similar overestimation of the gap at small U/t may also affect our results on 2D lattices. For larger U/t the accuracy improves rapidly as electron localization starts to set in, and the relative error in ΔE_{c} vanishes. Therefore, the development of a Mott insulator with increasing U/t is described correctly.

Finally, we would like to comment briefly on a few other applications: (i) Dimerized chains with hoppings $t \pm \delta t$ have been investigated by allowing for alternations of γ_{12} in Eq. (11). One observes that the precision of the results improves systematically with increasing dimerization. For example, for $N_a = N_e = 12$ and $U/t = 4$, we find $|E_{gs} - E_{gs}^{ex}|/|E_{gs}^{ex}| = 3.3 \times 10^{-2}$, 1.4×10^{-2}, and 2.6×10^{-3} for $\delta t/t = 0$, $1/2$, and $3/4$, respectively. The non-dimerized case, shown in detail in Fig. 2, is in fact the most difficult one, since for a collection of dimers

($\delta t = t$) the exact W is recovered [Eq. (10)]. (ii) Three dimensional (3D) lattices are a further interesting direction for future developments. Indeed, encouraging results have been obtained for the simple cubic lattice at half-band filling. LDFT with Eq. (11) for W yields $E_{gs}/t = 1.21$, 0.81, and 0.59 for $U/t = 4$, 8 and 12, respectively, in good agreement with corresponding quantum Monte Carlo results,[15] namely, $E_{gs}^{\mathrm{QMC}}/t = 1.27$, 0.78, and 0.57. (iii) An accurate approximation to $W(\gamma_{12})$ has been also derived for the attractive (negative U) Hubbard model in an analogous way as for $U > 0$. For a 1D ring with $N_a = N_e = 12$ we find $|E_{gs} - E_{gs}^{ex}|/|E_{gs}^{ex}| = 1.2 \times 10^{-3}$, 7.5×10^{-3}, and 1.5×10^{-4} for $|U|/t = 1$, 4, and 64, respectively. These results show that LDFT describes electronic correlations correctly also when intra-atomic pairing is favored. Systematic investigations along these lines are currently in progress and will be published elsewhere.[12]

V. CONCLUSION

A new density-functional approach to lattice-fermion models has been developed that is by all means independent of the homogeneous electron gas. A simple approximation to the interaction-energy functional is derived for the Hubbard model, which provides with a unified description of correlations in all interaction regimes from weak to strong coupling. Results for the ground-state energy and charge-excitation gap of 1D and 2D systems demonstrate the ability of lattice density functional theory to describe quantitatively the subtle competition between kinetic charge fluctuations and correlation-induced localization. The scope of DFT is thereby extended to the limit of strong electron correlations.

Several interesting directions open up with potential implications in various related areas. For example, one may explore more general approximations to $W[\gamma]$ and one may apply the present approach to richer physical situations such as low-symmetry systems, disorder, magnetic impurities, or multiband Hamiltonians. These developments should be relevant to the study of lattice fermion models and also in view of a DFT description of strong correlations from first-principles.

Acknowledgments

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